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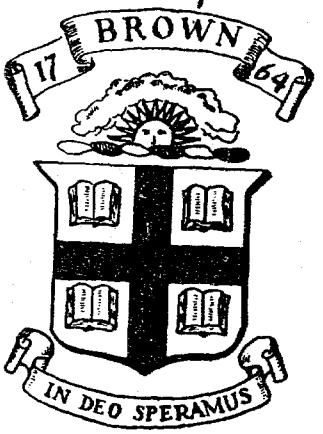

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THERMODYNAMICS OF A LOOSELY-PACKED GRANULAR AGGREGATE

BY

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FOREWORD

The present study is part of a program of "Theoretical Research on Combustion and Wave Propagation in Metal Dust-Oxidant Mixtures" being conducted by the Division of Engineering, Brown University, under United States Army Ordnance Contract No. DA-19-020-ORD-4761. The work was administered by the Pyrotechnics Laboratory of the Picattiny Arsenal, Dover, N. J.

SUMMARY

The thermodynamic properties of a loosely-packed granular aggregate are calculated. An application of these formulas to the study of a shock wave in a granular mixture is indicated.

THERMODYNAMICS OF A LOOSELY-PACKED GRANULAR AGGREGATE

1. Introduction

We shall be concerned with a loosely-packed granular aggregate, the space between the granules being filled with a perfect gas. We assume that the diameter of the individual granules is much smaller than the smallest macroscopic scale of interest and that in every macroscopic volume there are a large number of granules. Under such conditions the granular aggregate may be considered as a continuum from the macroscopic viewpoint.

The mechanical properties of such a continuum, of course, depends on the microscopic state of the granular aggregate. When the average distance between the neighboring granules is large compared to the average diameter of the granules, the medium behaves (from the macroscopic viewpoint) as a fluid. It is in fact a "dusty gas". The thermodynamics behavior of a dusty gas has been discussed in ref. 1.

Let us compress the medium (for example, by a piston) until the granules begin to pack together. Further compression will be resisted not only by the gas pressure but also by the granules. Since the elastic moduli of the granules are much higher than the elastic modulus of a gas, we may consider the granules as being rigid. Part of the energy expended in compressing the gas is stored up in the gas, the remaining part is expended against the friction between the granules and cannot be recovered. If the piston is now retracted by a very slight amount, the granules will no longer participate in exerting any force on the piston. The force on the piston required to maintain this small change drops sharply to a value equal to that contributed by the gas pressure. If we now recompress the medium, the granules will again participate in resisting the piston and the force required for this compression rises sharply. Further compression will ultimately cause the granules to lock into one another, the medium

then behaves as a porous rigid solid. The thermodynamics of a porous rigid solid may be deduced from that of a porous elastic solid which has been treated in ref. 2.

In this report, we shall examine the thermodynamics of a loosely-packed granular aggregate of rigid granules in the intermediary range between a "dusty gas" and a "porous rigid solid", a range in which the medium exhibits what is usually called "plastic deformation".

2. Entropy Production in a Deformation

We have seen that when our medium is compressed, part of the work done on the medium cannot be recovered. Of course, this is because work must be expended in overcoming intermolecular friction and is transformed into heat, resulting in a production of entropy inside the medium. In the present case the entropy produced can be easily calculated.

We begin by considering a cylinder containing a unit mass of the gross medium. At one end of the cylinder is a movable piston. Let us denote the area of this piston by A_p, the loading on it by σ (in force per unit area) and the height of the piston by χ. Part of the loading is carried by the granules; we shall denote this part by σ'. The remaining part, denoted by σ'', will be resisted by the pressure in the gas. Thus

$$\sigma = \sigma' + \sigma'' \tag{2.1}$$

This may also be illustrated in a stress-strain diagram. (See Fig. 2). Let σ_0 and χ_0 be the values of σ and χ when the medium just ceases to become a "dusty gas" at the temperature T_0. We introduce a measure of compressive strain defined by

$$\epsilon = 1 - \frac{\chi}{\chi_0} \tag{2.2}$$

In figure 2, we plot σ vs ϵ in an isothermal compression. ABC represents the loading curve, BDA represents a typical unloading curve.

The ordinate FB represents the total load σ ; the ordinate FD represents the part σ'' resisted by the gas while DB represents the part σ' .

The work done in compressing the gas is $\sigma A_p dx$ or $-\sigma dV$ where dV is the increase in volume of the cylinder. Thus, a positive work is expended when the volume decreases. The work stored in the gas is $-\sigma'' dV$ and that transformed into heat is $-\sigma' dV$. Hence the entropy produced in a compression per unit mass of the gross material is

$$dS_i = -\frac{\sigma' dV}{T} \tag{2.3}$$

where dV is clearly the specific volume of the material. Note that this formula applies only if $dV < 0$, since the unloading process is reversible.

An estimate of the entropy produced in a deformation can be easily made if the work done in compressing the material is given and the composition, density and temperature of the mixture are known. The composition of the material may be conveniently described by the mass fraction Y' of the granules in the gross material. Or it may be described in terms of the mass fraction Y'' of gas in the gross material. Of course

$$Y' + Y'' = 1 \tag{2.4}$$

Furthermore, if the density of the granules is ρ' , which is assumed known, the total volume occupied by the granules in the mixture is Y'/ρ' . The total volume occupied by gas in the mixture is then $V - Y'/\rho'$ consequently, by the gas law,

$$\sigma'' = RT/(V - Y'/\rho') \tag{2.5}$$

where R is the gas constant and T is the temperature of the medium. The entropy produced in a deformation is:

$$dS_i = \frac{dw}{T} - \frac{R dV}{V - Y'/\rho'} \tag{2.6}$$

where dw is the work done in compressing the material.

3. A Fundamental Relation

The first law of thermodynamics states that

$$dQ + dW = dU \tag{3.1}$$

where dQ is the heat added to the material and dU is the internal energy per unit mass. If dS_e denotes the entropy added to the material as a result of heat transfer to the medium,

$$dQ = T dS_e \tag{3.2}$$

But

$$dW = -\sigma dV = -\sigma'' dV + T dS_i \tag{3.3}$$

therefore:

$$T(dS_e + dS_i) = dU + \sigma'' dV \tag{3.4}$$

Now $dS = dS_e + dS_i$, therefore

$$T dS = dU + \sigma'' dV \tag{3.5}$$

Introducing Helmholtz force energy per unit mass of the gross material,

$$A = U - TS \tag{3.6}$$

we have

$$dA = -S dT - \sigma'' dV \tag{3.7}$$

Consequently,

$$\sigma'' = -\frac{\partial A}{\partial V} \tag{3.8}$$

$$S = -\frac{\partial A}{\partial T} \tag{3.9}$$

$$U = A - T\frac{\partial A}{\partial T} \tag{3.10}$$

4. Internal Energy and Entropy of The Material

From (2.5) and (3.8) we have

$$-\frac{\partial A}{\partial V} = \frac{RT}{V - Y'/\rho'} \tag{4.1}$$

Since γ'/ρ' is the volume occupied by the granules in a unit mass of the gross material, it is convenient to introduce the notation

$$v_g = \gamma'/\rho' \tag{4.2}$$

Integrating (4.1), we obtain

$$A - A_0 = -RT \log_e \left(\frac{V - v_g}{V_0 - v_g}\right) + \alpha(T) \tag{4.3}$$

where A_0 and V_0 are the values of A and V when $T = T_0$ and $X = X_0$, (cf. eq. 2.2). $\alpha(T)$ in (4.3) is an arbitrary function satisfying the condition $\alpha(T_0) = 0$. Substituting (4.3) into (3.9) and (3.10) we find:

$$S = R \log_e \left(\frac{V - v_g}{V_0 - v_g}\right) - \frac{d\alpha}{dT} \tag{4.4}$$

and

$$U = A_0 + \alpha(T) - T\frac{d\alpha(T)}{dT} \tag{4.5}$$

Thus, the internal energy of our material is a function of T only. This is as it should be, because

$$U = \gamma' U' + \gamma'' U'' \tag{4.6}$$

and the internal energy U' of the rigid granules and U'' of the gas are both function of T. $\alpha(T)$ can now be calculated from (4.5) and (4.6). Thus,

$$\alpha(T) = A_0 \frac{T - T_0}{T_0} - T\int_{T_0}^{T} \frac{U(T)}{T^2} dT \tag{4.7}$$

5. Shock Wave in A Loosely-Packed Granular Medium

As a simple application, the forgoing thermodynamic formulas may be applied to calculate the discontinuous change of state across a shock wave in a loosely-packed granular medium. Of course, we shall also need an expression for the variation of the stress component σ' with strain ϵ. A relation between σ' and ϵ can, in principle, be determined

experimentally by carrying out a compression test of the material in an evacuated container. In general, a relation of the type

$$\sigma' = F(\epsilon) \tag{5.1}$$

can be expected where $F(\epsilon)$ is independent of the temperature T, provided that T is much smaller than the melting point of the granules. Furthermore, we assume that $F(0) = 0$ and $F(\epsilon) \to \infty$ as $\epsilon \to \epsilon^*$, at which point the granules are so tightly-packed that no further deformation is possible without cracking them. As a rough approximate a σ' vs ϵ curve of the form shown in Fig. 3 may be used.

The basic equations governing the jump across a shock wave are then:

$$\rho_2 u_2 = \rho_1 u_1 \tag{5.2}$$

$$\sigma_2 + \rho_2 u_2^2 = \sigma_1 + \rho_1 u_1^2 \tag{5.3}$$

$$U_2 + \frac{\sigma_2}{\rho_2} + \frac{1}{2} u_2^2 = U_1 + \frac{\sigma_1}{\rho_1} + \frac{1}{2} u_1^2 \tag{5.4}$$

$$U = U(T) \tag{5.5}$$

$$\sigma = \sigma' + \sigma'' \tag{5.6}$$

$$\sigma' = F(1 - \rho_0/\rho) \tag{5.7}$$

$$\sigma'' = RT/(V - V_g) \tag{5.8}$$

where subscripts "1" and "2" refer respectively to the conditions ahead of and behind the shock, ρ denotes the density of the gross material and u denotes the velocity. Eqs. (5.2), (5.3) and (5.4) are respectively the continuity, momentum and energy equations; eqs. (5.5) and (5.8) are the equations of state, while (5.7) describes the irreversible part of the stress-strain relation.

If we substitute eqs. (5.5), (5.6), (5.7), (5.8) into (5.2), (5.3), (5.4), we obtain a system of three equations involving ρ_2, u_2 and T_2.

Solving these in terms of σ_1, ξ_1, u_1 and T_1, the dynamic state of the material behind the shock is completely determined. In particular, σ_2 can be computed from (5.6).

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2. Chu, B. T., "Thermodynamics of a Porous Elastic Solid Containing A Compressible Fluid". Brown University Rpt. DA-4761/2 June, 1960. Department of Army Project No. 5S04-01-027. Ordnance R and D Project No. TS5-5407N. Contract No. DA-19-020-ORD-4761.

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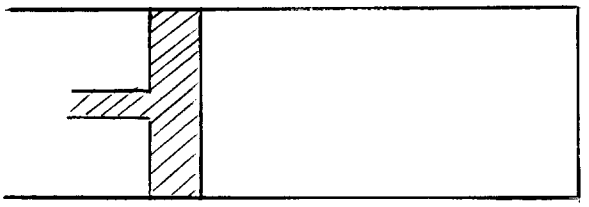

Figure 1

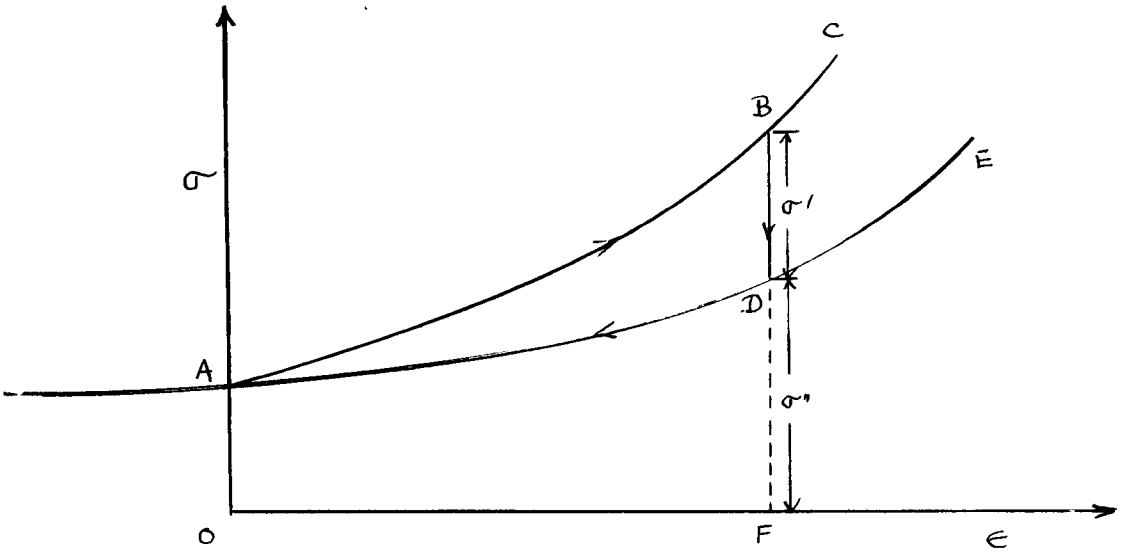

Figure 2

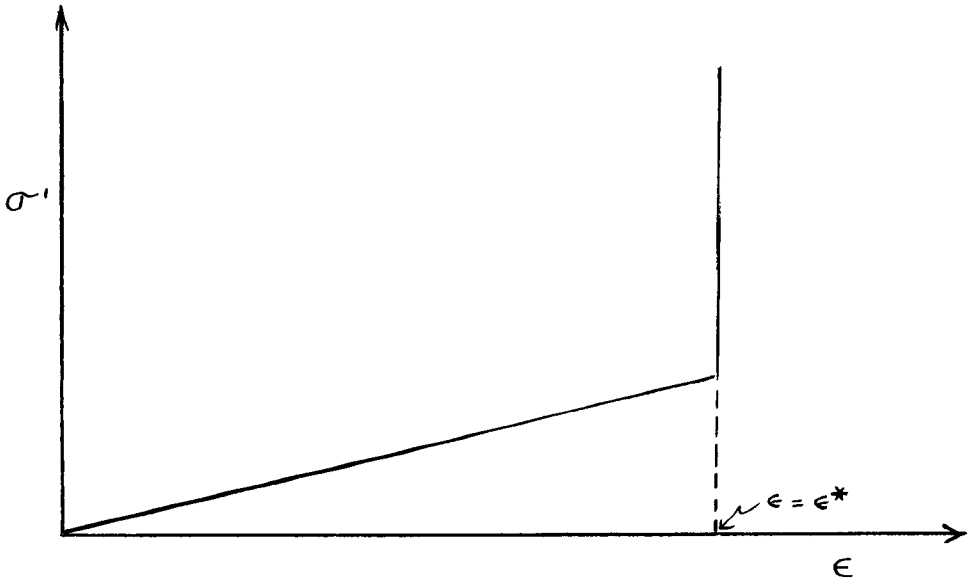

Figure 3